

Identification of the Selective Sites for Electrochemical Reduction of CO to C₂+ Products on Copper Nanoparticles by Combining Reactive Force Fields, Density Functional Theory, and Machine Learning— Supporting Information

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S1. Methods

S1.1 ReaxFF

The copper nanoparticle investigated in this study is computationally synthesized in the same way as in [1]. The embedded-atom model (EAM) [2] was used to model the interactions between copper atoms. To simulate the chemical vapor deposition (CVD) synthesis, copper atoms are added to the simulation box in a rate of 3.2A/ns for 30ns. After the nanoparticle condenses, a total of 38 simulated annealing cycles is applied to relax the initially formed structure. Each cycle involves a heating step from 300K to 1200K in 5ps, high temperature step at 1200K for 5ps, cooling step from 1200K to 300K in 5ps, and room temperature step at 300K. At last, the final copper nanoparticle is relaxed using the reactive force field [3] at 300K for 20ps.

S1.2 DFT

The density functional theory (DFT) calculations are performed in VASP [4]. The PBE functional [5] is used to obtain electronic energy. The plane wave basis up to a kinetic energy cutoff of 400eV is used to describe the wave function. Since copper is metallic, the method of Methfessel-Paxton of order 1 is used for smearing. The smearing width is 0.2eV. The convergence criteria for electronic energies is 1e-5eV, and the geometries are optimized until the force converged to be within an error of 0.01eV/Å.

ΔE_{CO} and ΔE_{OCCOH} are calculated in the same way as in [1]:

$$\Delta E_{CO} = E[*CO] - E[*] - E[CO]$$

$$\Delta E_{OCCOH} = E[*OCCOH] - E[*CO, *CO] - 0.5 \times E[H_2]$$

S1.3 Neural Network Machine Learning Model

The neural network used in this study is of the type by Behler and Parrinello [6]. However, instead of summing up contributions from all atoms, only the contribution from the target surface atom is

used. In this study, instead of the atomic energy, the quantity to be fitted using machine learning is the CO adsorption energy.

As we have shown earlier [1, 7], the CO adsorption energy can be sufficiently described on the surface of the nanoparticle by considering all the atoms within 8Å of the surface site. Thus, a copper cluster of 8Å radius about each surface atom is extracted from the nanoparticle to compute the CO adsorption energy. Subsequently, the same cluster is used as the input to the machine learning model. Since we are only considering the chemical behavior of the chosen surface site, only molecular descriptions about that site are used as input to the neural network. Similar to our previous model, two-body and three-body features are used. The overall structure of the neural network machine learning model is shown as below:

And mathematically, the above model is represented as follows:

$$G_{i\alpha}^{(2)} = \sum_j \phi_{\alpha}^{(2)}(\mathbf{p}_{ij}), G_{i\beta}^{(3)} = \sum_{jk} \phi_{\beta}^{(3)}(\mathbf{p}_{ij}, \mathbf{q}_{ijk}) \quad (1)$$

$$E_{CO} = F_{NN}(\{G_{i\alpha}^{(2)}, G_{i\beta}^{(3)}\}; \mathbf{w}, \mathbf{b}) \quad (2)$$

Where $G_{i\alpha}^{(2)}$ and $G_{i\beta}^{(3)}$ are the 2- and 3-body descriptors from the 2- and 3-body geometrical features \mathbf{p}_{ij} and \mathbf{q}_{ijk} , e.g., the 2-body term can include the interatomic distance $p_{ij} = R_{ij}$, and the 3-body term can include the angle formed by three atoms $q_{ijk} = \theta_{ijk}$. Finally, the function $F_{NN}(\mathbf{G}; \mathbf{w}, \mathbf{b})$ represents the network network that transforms the input descriptors \mathbf{G} into a single value using the parameters with weights \mathbf{w} and biases \mathbf{b} . The final value calculated from the whole model is the CO adsorption energy, as represented by equation (2).

The molecular descriptors as input to the neural network can be extracted in many ways. In this study, the set of piecewise cosine function is used because it is a more systematic way of constructing locally based symmetry functions.

$$R_{\alpha}^k = R_{inner} + (\alpha - 1)h_k \quad \text{where } \alpha = 1, 2, \dots, M_k$$

$$\varphi_{\alpha}^{(k)}(R_{ml}) = \begin{cases} \frac{1}{2} \cos\left(\frac{R_{ml} - R_{\alpha}^k}{h_k} \pi\right) + \frac{1}{2}, & |R_{ml} - R_{\alpha}^k| < h_k \\ 0, & \text{Otherwise} \end{cases} \quad (3)$$

$$G_{\alpha,l}^{(2)} = \sum_m \varphi_{\alpha}^{(2)}(R_{ml}) \quad (4)$$

$$G_{\alpha\beta\gamma,l}^{(3)} = \sum_{m,n} \varphi_{\alpha}^{(3)}(R_{ml}) \varphi_{\beta}^{(3)}(R_{nl}) \varphi_{\gamma}^{(3)}(R_{mn}) \quad (5)$$

where:

$\varphi_{\alpha}^{(k)}(R_{ml})$ is the piecewise cosine function over the interatomic distance R_{ml}
 $k=2,3$ corresponds the 2-body and 3-body terms, and

$h_k = (R_{\text{outer}} - R_{\text{inner}})/M_k$ is the width of the piecewise cosine functions.

The set of piecewise cosine functions are described by 4 quantities, the inner cutoff R_{inner} , the outer cutoff R_{outer} , the number of two-body functions M_2 , and the number of three-body functions M_3 . Here, the $M_2=12$ and $M_3=3$ are used, corresponding to a set of 30 unique descriptors for each copper cluster. Because each cluster is only of 8 angstroms, we can include all the atoms in the descriptor. Thus, R_{outer} is set to 8Å. Since only 12 two-body functions are used, the width of each piecewise cosine function is relatively large, thus, R_{inner} can be set to 0. Once the input atomic descriptors are assembled about the target surface site, it was fed through a two-layer neural network each with 50 nodes to produce one output, which is then fitted to the adsorption energy.

S2. Implementation and Training of the Neural Network Model

The above neural network is implemented in Python and is freely available on our Gitlab page at: https://gitlab.com/yufeng.huang/cunp_coads. Instructions on how to use the neural network model is described on the website.

Once the structure of the neural network is constructed, the weights and biases of the neural network model are initialized using the Xavier initializer [8]. Then using the 8:1:1 split of the data set for training, validation and testing, we obtain the following RMSE as a function of training iterations, as shown in Figure S2(a). The final RMSE of the training set, validation set, and test set are 0.111eV, 0.117eV and 0.123eV. The overall distributions between the DFT energies and the neural network predicted values also agree, as shown in Figure S2(b).

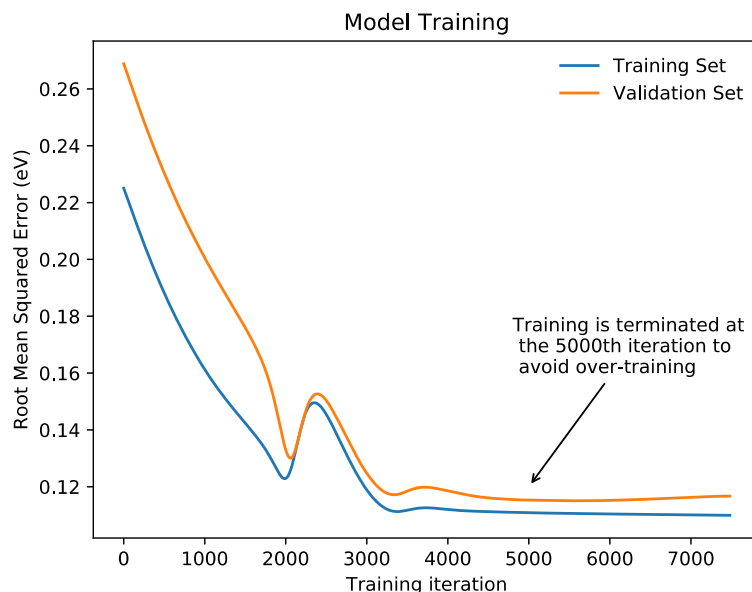


Figure S1. RMSE of the training set and validation set as functions of the training iterations.

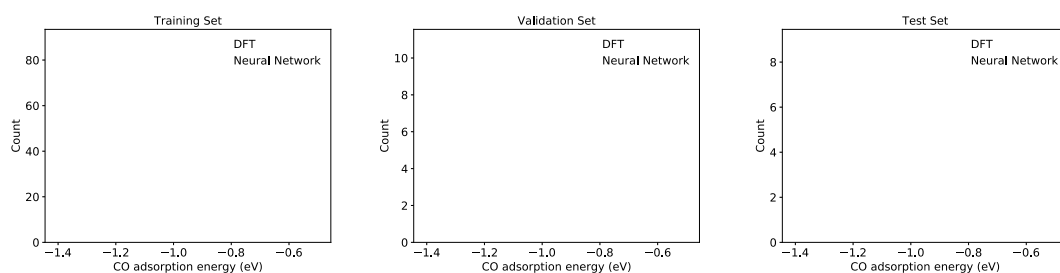


Figure S2. Distribution of the energies between the DFT values and the neural network predicted values for the training set, validation set, and the test set.

Unit: eV	DFT range	NN range
Training Set	[-1.284, -0.458]	[-1.262, -0.715]
Validation Set	[-1.276, -0.543]	[-1.158, -0.820]
Test Set	[-1.314, -0.433]	[-1.278, -0.761]

Table S1. Energy ranges between DFT and neural network for the training set, validation set, and test set. Because CO does not adsorb on certain unfavorable sites, these sites are treated as high adsorption energies. Due to this, the upper end of the range has much larger error to include the unfavorable outliers than the lower end. However, NN predicts the lower end of the ranges very well, indicating that good CO adsorption sites are well identified.

NN sizes	Training set RMSE	Validation set RMSE	Test set RMSE
30x2	0.110 eV	0.123	0.140
40x2	0.115	0.118	0.135
50x2	0.108	0.119	0.122
60x2	0.103	0.116	0.117

Table S2. RMSEs of the training set, validation set, and test set as functions of the neural network sizes. The notation $nx2$ indicates two hidden layers with n nodes are used in the neural network. Although the training set and validation set are fitted in similar accuracies between different sizes, the test set error is smaller when the size of the neural network increases. The neural network size of 50x2 is used to allow enough flexibility.

S3. Relationship between E_{OCCOH} and C_2 products selectivity

Hori et al. (2002) [9] reported the selectivity for C_2 products on different crystalline surfaces of copper. Using their reported values and our theoretical $^*\text{OCCOH}$ reaction energy, E_{OCCOH} , we found that the log of the ratio between C_2H_4 and CH_4 correlates almost linearly E_{OCCOH} , as shown in the following figure. This is not surprising because the reaction rates are typically exponentially dependent on energy as in the Eyring equation or Arrhenius equation. However, the good fit

between the selectivity and E_{OCCOH} implies that E_{OCCOH} is a good descriptor for the selectivity of C_2 products.

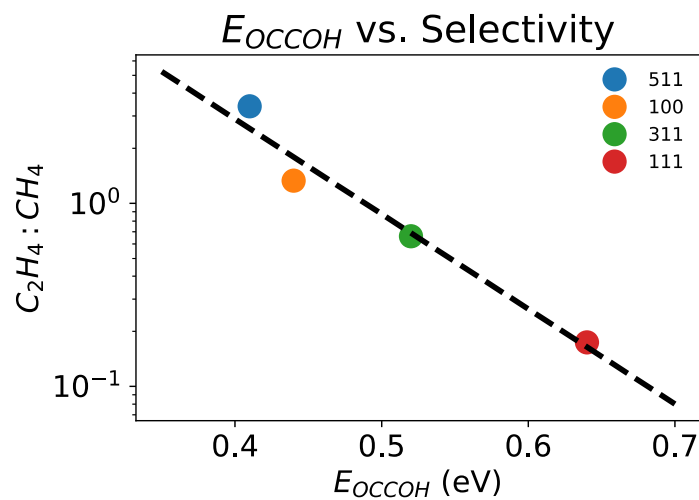


Figure S3. Experimental $\text{C}_2\text{H}_4:\text{CH}_4$ ratio and the reaction energy of E_{OCCOH} . Note, the logarithm of the ratios is used for the y-axis.

S4. Surface terminations of the Twin boundaries

Based on the configurations of the adsorbed $\ast\text{OCCOH}$ on the copper clusters, there are 4 ways of placing the intermediate on the surface, as shown in the following figure, Figure S4. This is due to two factors. First, the (100) surfaces intersecting at the twin boundary can be concave or convex, as indicated by the purple figure in Figure 4(a) in the main text and the side view in Figure S4. Second, the plane formed by the adsorbed $\ast\text{OCCOH}$ can be in the same plane as the page, or perpendicular to the page, as shown in top view in Figure S4.

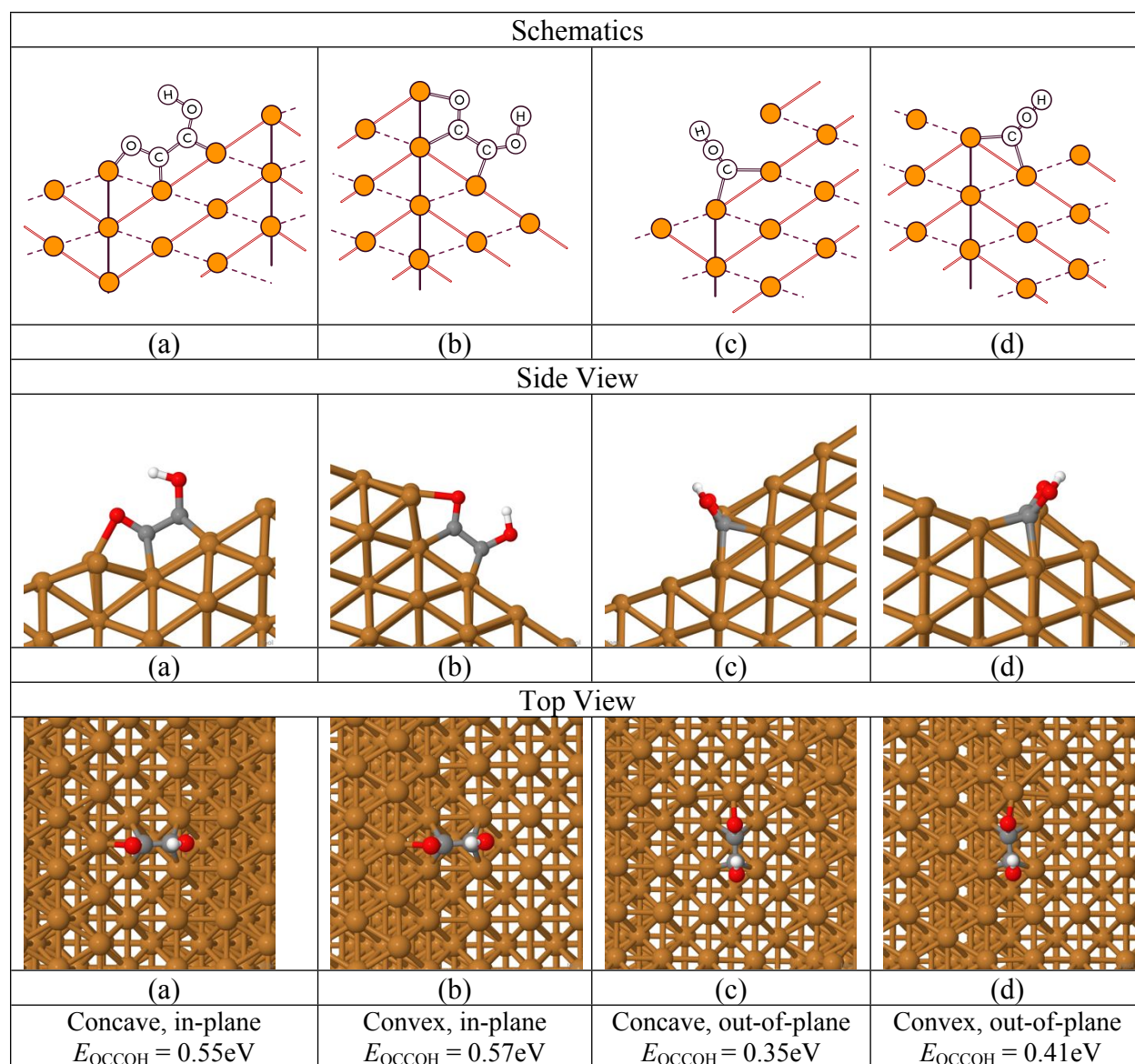


Figure S4. The four configurations of $\ast\text{OCCOH}$ binding at the twin boundary of copper. (a): $\ast\text{OCCOH}$ adsorbed in-plane at the concave site; (b): $\ast\text{OCCOH}$ adsorbed in-plane at the convex site; (c) $\ast\text{OCCOH}$ adsorbed out-of-plane at the concave site; (d) $\ast\text{OCCOH}$ adsorbed out-of-plane at the convex site.

S5. Prediction of Faradaic Efficiencies

The data for currents J_{C2+} and J_{H2} as functions of the grain boundary density d_{GB} are obtained from Figure 3(d) and (g) of reference [10]. First, since J_{H2} does not depend on d_{GB} , and the terminal value is 3.1 mA/cm² for large d_{GB} , we then keep J_{H2} constant for this approximation. For C₂₊ production, J_{C2+} is fitted linearly as in the experimental data. Then we have:

$$J_{C2+} = 0.18 * d_{GB} - 0.399$$

$$J_{H2} = 0.31$$

Where d_{GB} is in units of μm^{-1} , J_{C2+} and J_{H2} are in units of mA/cm².

Our periodic structure has twin boundary density of 649.5 μm^{-1} . Thus, the faradaic efficiency is then $J_{C2+} / (J_{C2+} + J_{H2}) = 97.4\%$

Also, [11] reported a copper structure with a large abundance of twin boundary sites with spacing of 5~70nm, which corresponds to densities of 14.3 to 200 μm^{-1} . The corresponding faradaic efficiencies are 41.2% to 92.0%.

The results are summarized in Figure 5 of the main text.

S6. Coordinates of the structures used in this study

Cu(511) *OCCOH

1.0000000000000000

10.2671904600000001 0.0000000000000000 0.0000000000000000

-3.8501964300000000 6.6687358249999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C H

44 2 2 1

Direct

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0.1553998011691154 0.5248760836634501 0.2115957196888001
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0.9045966398543442 0.5240951004183302 0.2126142380767774
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0.5538792031590452 0.5728369919438520 0.5113004170087873

Cu(511) *COCO

1.0000000000000000

10.2671904600000001	0.0000000000000000	0.0000000000000000
-3.8501964300000000	6.6687358249999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Cu O C

44 2 2

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0.2556211801116567	0.7497392599609557	0.3788945367972170
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Cu((100) *OCCOH

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0.0000000000000000 10.2671904600000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C H

64 2 2 1

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0.8053736811710399 0.1890948306676656 0.2370434468043215
0.8020653780668966 0.4377643586365473 0.2387408988069600
0.8040279751216436 0.6861368089024462 0.2376164096355655
0.8061908716259002 0.9385012816239130 0.2362329675702796
0.1810450663558177 0.0624579153090253 0.1632107395493586
0.1810258940926406 0.3124950140609346 0.1634989370476813
0.1811830155232740 0.5626418758218855 0.1638614657833896
0.1812339985212833 0.8125819331436157 0.1636485608727600
0.4306874649786389 0.0628779454841173 0.1631280457611556
0.4304540144305393 0.3124257191030486 0.1632465817912415
0.4304996861832777 0.5626755574615641 0.1636023944583785
0.4304683901657916 0.8131036669268437 0.1631026510880138
0.6813253674135290 0.0628595948651386 0.1631036102758778
0.6813288643886309 0.3124087626355639 0.1632277547940076
0.6812722128260426 0.5626530516913997 0.1635921328610091
0.6814874818328031 0.8130964112070121 0.1630821081016773
0.9309413169388382 0.0624450951921121 0.1631938103153384
0.9307154991319987 0.3124801807284585 0.1634943284343389
0.9305746872022664 0.5626226588511202 0.1638538443276547
0.9307357625554185 0.8125646277039867 0.1636362016474673
0.0562850024445198 0.1875867747740034 0.0921436209835136
0.0560507191927593 0.4381872186480217 0.0928598399363762
0.0561538114919837 0.6877857132568569 0.0929054302259138
0.0565117374901673 0.9382856358819004 0.0917666173927871

0.3055812314680610	0.1875791690818680	0.0919846322217848
0.3057080511837387	0.4383299274950464	0.0928125805779383
0.3057690046670202	0.6880591001730368	0.0924726083148694
0.3060183403670710	0.9383749618335530	0.0918816076003223
0.5562140614331338	0.1879265139640544	0.0926835160188537
0.5560249341356287	0.4384533585448865	0.0931840553175545
0.5561324533064169	0.6879994303795844	0.0930004842042443
0.5564306532055193	0.9382361962184048	0.0921478523258709
0.8069645893458303	0.1875659697604400	0.0919404356864950
0.8063834944467198	0.4383040463319802	0.0927926982241767
0.8065436256696327	0.6880337524972026	0.0924497543198362
0.8069180545401317	0.9383589085627806	0.0918450058304251
0.5563349956275088	0.5693510695713069	0.4167642583358337
0.5552934801291808	0.3027895285323647	0.4173044215489352
0.5554787898074516	0.3608442642973005	0.3735942592412904
0.5559440575253547	0.5041589362260730	0.3686533765791161
0.5558867835572097	0.5027132308986797	0.4452476377406138

Cu(100) *COCO

1.0000000000000000

10.2671904600000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2671904600000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Cu O C

64 2 2

Direct

0.1803894877443313	0.0614995534602743	0.3065465325040224
0.1789147936936173	0.3129970796052410	0.3069355611121988
0.1806318364173024	0.5627077720705843	0.3065043539539196
0.1813124037462196	0.8117340173942427	0.3064972715112103
0.4315149552205801	0.0608085360920075	0.3067958158065053
0.4301800685226396	0.3131406837270845	0.3120961843417546
0.4290305071582139	0.5653321950627352	0.3074710654736365
0.4302563966616144	0.8136586708296968	0.3062378360136146
0.6812754860006657	0.0612930634759451	0.3061975452672966
0.6828614158107962	0.3098889349746843	0.3074331000324027
0.6815652007084292	0.5618775409229920	0.3121662787499035
0.6800642981047561	0.8142121264740159	0.3068571232727522
0.9302028073263006	0.0627510155353754	0.3065060983875504

0.9310517772325280 0.3117861983111581 0.3064779373717925
0.9328670487292627 0.5615864048906882 0.3069456433873871
0.9311273838100471 0.8130315444105018 0.3065747582283588
0.0561350742429112 0.1881760595476752 0.2357916384062753
0.0559931782157336 0.4376209461380758 0.2356996146259350
0.0557552662608272 0.6870355599158480 0.2357960024682210
0.0559281178419732 0.9375991204393884 0.2357580747108962
0.3073382513605915 0.1890501269027911 0.2367763060622653
0.3079694283715163 0.4367718304980522 0.2368913147958931
0.3066898713027598 0.6870275550999670 0.2357522218159134
0.3063188503290909 0.9381289978445304 0.2355837372778087
0.5555321559633352 0.1889541879265572 0.2363767580116601
0.5561070571350087 0.4378679543281436 0.2376694091546973
0.5564343052951125 0.6865851076976347 0.2363851598653481
0.5559590431847269 0.9377387123022548 0.2355530611025451
0.8052456663876971 0.1882874338085879 0.2357382383930349
0.8040980912021021 0.4385787289296957 0.2368558669011225
0.8045497939666181 0.6862113615072010 0.2367537725826981
0.8055801477779675 0.9371670946429148 0.2355909709061174
0.1808986566549882 0.0627061729824455 0.1626751465067024
0.1812234544332486 0.3119488328976660 0.1626369047994245
0.1810356210238782 0.5623412450972562 0.1626898118624797
0.1803416669838983 0.8129062222112320 0.1627245250427100
0.4303356812072312 0.0628628751445156 0.1624572910509974
0.4309026214042822 0.3126136855151907 0.1627402685600511
0.4310566933150681 0.5622000129476645 0.1624277337481939
0.4308949039356332 0.8124954919756670 0.1624520303328303
0.6809998926075423 0.0624974549289437 0.1624489409065777
0.6808063018985444 0.3128234194263205 0.1624092057159560
0.6809391938684710 0.5623989937226554 0.1627082895192255
0.6815510907263136 0.8121141420185849 0.1624511343683545
0.9315257550137653 0.0619971814815180 0.1627070883687356
0.9308120416084724 0.3125702816248667 0.1626664116862480
0.9306082633785987 0.5629883027837100 0.1626160662523605
0.9309498538091796 0.8122159941599542 0.1626744268201449
0.0572682174774231 0.1869351975166207 0.0914352487915656
0.0561937187900700 0.4379544057509239 0.0922541599701151
0.0552945185179107 0.6890015910037927 0.0914372276493757
0.0563270080305984 0.9379974430726454 0.0906743523879562
0.3053861657993510 0.1874328694740842 0.0912871098226517

0.3061477677544631	0.4375753420815399	0.0921114215836917
0.3057841439965676	0.6881529523585392	0.0922362225560484
0.3047579476105755	0.9389282364218630	0.0913953724872644
0.5557858103787731	0.1881505861994923	0.0921352101647186
0.5561905625620162	0.4379587230379372	0.0920552393765490
0.5566769975757493	0.6877682362335222	0.0921094297556652
0.5562553311802630	0.9379503961040986	0.0921905270663067
0.8066520162300799	0.1877507330037198	0.0922135951684225
0.8062504224563386	0.4383634688295555	0.0920739336547410
0.8072081885819092	0.6885765280266131	0.0912441803991406
0.8077711178052458	0.9370297584709758	0.0913830613381683
0.6609444531390327	0.5954501839338852	0.4315436350179352
0.4504730505641419	0.2788074824700980	0.4314474697095574
0.4427876461912461	0.2936234986029457	0.3856091219685472
0.6687269750675582	0.5808752124157099	0.3856976077955634

Cu(311) *OCCOH

1.0000000000000000

10.2671904600000001	0.0000000000000000	0.0000000000000000
-2.5667976200000000	8.5131046000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Cu O C H

64 2 2 1

Direct

0.1078279995622055	0.2004791637780104	0.3478154963026278
0.1127777717205317	0.7054062559359431	0.3467064138633793
0.3588047730241782	0.1790336389292485	0.3525397580616469
0.3651659714027547	0.7080756089640579	0.3527707839120249
0.6189006825747934	0.1983965256349440	0.3468947043804874
0.6150059556740203	0.7113247770215997	0.3528067349369092
0.8655662647303783	0.2076243703237749	0.3467213557121775
0.8637984999587910	0.7058220740135451	0.3469310499243108
0.0475705220064718	0.4321963686638257	0.3099581281682567
0.0465345558411820	0.9315668969415746	0.3097015354414377
0.2989550237588315	0.4305883443998902	0.3140871606124626
0.2958378195452130	0.9252602644198253	0.3084524440258049
0.5449576823592581	0.4325771173798402	0.3146170772847703
0.5446833092241120	0.9300796826529748	0.3077109328358320
0.7962887166894705	0.4328923664382247	0.3095798489627161

0.7950723573885385 0.9320754272874487 0.3114675821931810
0.2286365353638967 0.1557015546742712 0.2652907060757720
0.2292553720202375 0.6542064024912969 0.2660164673703785
0.4746037368695061 0.1570934711061282 0.2649047829010985
0.4766675706693596 0.6568849473156974 0.2633466744544340
0.7266011508621001 0.1563357495462578 0.2631239100167053
0.7230398574614265 0.6561075679310048 0.2663497338787753
0.9771863541882631 0.1551039029860640 0.2637539466379415
0.9765493439874947 0.6548863602879420 0.2637308043980781
0.1623549632765516 0.3882488762558621 0.2232525702722496
0.1576782945067456 0.8858173622966460 0.2212861625289473
0.4088192460216214 0.3875434051474769 0.2223179784956733
0.4078249778354166 0.8853662865195767 0.2214224094746039
0.6560243051184863 0.3884680573177784 0.2237756000494194
0.6585651642192415 0.8856773343707638 0.2215960088786961
0.9093523581854133 0.3878475186539689 0.2208386540377004
0.9083476257497057 0.8867071157918207 0.2216297739187206
0.0934422181008070 0.1176732938523778 0.1778423513667318
0.0949671846824819 0.6175491083109272 0.1777209133282789
0.3428979284046907 0.1182081798663074 0.1766036012016866
0.3431702048706916 0.6170449025410663 0.1769673150446529
0.5919232840493721 0.1178100997804533 0.1775629174679818
0.5939927685054830 0.6183842641310879 0.1772467205787567
0.8436931462900024 0.1186436552747681 0.1763292705533540
0.8416368586161868 0.6182387003870231 0.1780209831536266
0.0266576380813187 0.3490626776329026 0.1352807328385845
0.0249892069029060 0.8484796738073404 0.1351134533757622
0.2756061625617994 0.3497258730692001 0.1353951436610793
0.2760188378676048 0.8498383930238765 0.1349860645092363
0.5259352783673976 0.3507231830458844 0.1353816109313999
0.5255508802283655 0.8497955309042152 0.1349974715148387
0.7742365122439074 0.3500451872468563 0.1356056450405443
0.7758170486248399 0.8503896141245313 0.1348985065424243
0.2038150843366073 0.0724852309227317 0.0875604908126249
0.2048008527969341 0.5715967899804321 0.0880271982662836
0.4550377153165307 0.0732673763915300 0.0876587968224720
0.4560120935656909 0.5734187217245876 0.0885827449272454
0.7047643745013155 0.0739043314295347 0.0876301518113523
0.7060682937773675 0.5736565922465030 0.0883085098987862
0.9547843633219092 0.0723318661595976 0.0869646014334026

0.9551582843063933	0.5727403133803673	0.0885004994138711
0.1363248541479281	0.2995153294571151	0.0508621151073580
0.1371106600580292	0.7999205611868925	0.0516303049780426
0.3864927210722471	0.3006985889159239	0.0517156701083806
0.3868657047479491	0.7988925299881061	0.0513703372497243
0.6366485739595472	0.3012399873374552	0.0513428924483380
0.6376182088303269	0.8003491728373723	0.0513511750527492
0.8874731292227045	0.3015844367118958	0.0517518705497365
0.8875381444458305	0.8002685204072723	0.0510966900305390
0.3931120174688878	0.3229507176049723	0.4148103190692891
0.4723710573682723	0.6244760049671348	0.4570633382790956
0.4230717037645555	0.4460729840651288	0.3826953322347109
0.4642459944234939	0.6029412963031396	0.4026289967023141
0.4489340321104042	0.5194801721056154	0.4736799081556018

Cu(311) *COCO

1.0000000000000000

10.2671904600000001 0.0000000000000000 0.0000000000000000

-2.5667976200000000 8.5131046000000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C

64 2 2

Direct

0.1130595007964868	0.2066206571113990	0.3473078685704344
0.1124402113238278	0.7065236454735045	0.3469540417925046
0.3646213191815537	0.2032303599155708	0.3511361766775158
0.3617341302186995	0.7044029766453402	0.3472748382653399
0.6103339499234224	0.2053916481300105	0.3517730762394792
0.6126033383752585	0.7021086670669803	0.3521041065233747
0.8610769162516323	0.2069314344955722	0.3474105560703993
0.8627802891964743	0.7053370967442015	0.3469849650104419
0.0438288623858905	0.4330541860815227	0.3094405618034747
0.0444197960980104	0.9335464969061665	0.3098874270668089
0.2946997373003560	0.4306229821858295	0.3093113840871368
0.2938219343261291	0.9318548674245641	0.3091213158203152
0.5435082219844201	0.4344865683971122	0.3078787004111932
0.5432376206236601	0.9330108561041032	0.3084542916144212
0.7917075068988657	0.4320396902347476	0.3095244080188792
0.7930029305393264	0.9333592111654374	0.3097577810861889

0.2260366464128905 0.1576162082850971 0.2649174498938335
0.2235484227955051 0.6560552068869779 0.2634327864993120
0.4734090348709135 0.1577335281192088 0.2622349910335687
0.4742687399582400 0.6587277258238697 0.2636936521365292
0.7209890817810319 0.1589860627982458 0.2653564978566610
0.7212450386979845 0.6591850987897526 0.2647285519839576
0.9731015477682008 0.1569776608278050 0.2638712075728773
0.9732686757519760 0.6558913962137329 0.2633802064868712
0.1558130733177410 0.3888680551456653 0.2210527643906208
0.1559827400650779 0.8890828984364730 0.2207345756260572
0.4052993518695336 0.3889455476585399 0.2204761685061698
0.4048300737714954 0.8892358139848127 0.2204649383582697
0.6556190708359272 0.3888581938634598 0.2207887210469385
0.6555598491608529 0.8889404634328877 0.2214030986264724
0.9047328927620246 0.3889341707914131 0.2209964546583533
0.9056461566845623 0.8893987388930347 0.2207614300811606
0.0902975519097411 0.1193115206332249 0.1768353572521678
0.0898366939575239 0.6190779506586548 0.1763944270689216
0.3394672298202546 0.1193255411235233 0.1759398219133878
0.3400774282662281 0.6193705847730759 0.1763402037597153
0.5909944747045063 0.1196709866155052 0.1761489519973221
0.5904007068572705 0.6192486557050425 0.1760994730686054
0.8390908247125362 0.1201336280908890 0.1772253481857323
0.8387419108440551 0.6198315065399934 0.1765674693781778
0.0211508702615915 0.3501502601371385 0.1342497665442476
0.0218181890791267 0.8505465354337884 0.1341998616866503
0.2715982576564598 0.3509273589302154 0.1341423738905327
0.2714937730696083 0.8508079617989991 0.1338263759211743
0.5229943831732925 0.3516609503684573 0.1341755309395796
0.5226449318532440 0.8516385058410197 0.1343490613490713
0.7725405728068946 0.3522022318314617 0.1337705477347962
0.7723234143764057 0.8526151082559963 0.1343172765352045
0.2004095849501212 0.0728570206616128 0.0869456470088490
0.2003211483855348 0.5730619926027679 0.0867452564198054
0.4512580682570654 0.0735812251919506 0.0869833961038313
0.4507670046823691 0.5737541305626482 0.0871720968266791
0.7029408378814039 0.0759378453130767 0.0873002128631091
0.7023008622347212 0.5750941703576299 0.0869814797220577
0.9509121856667868 0.0752974607310972 0.0873152447237026
0.9511393289399647 0.5747368438029613 0.0867098014471671

0.1333430038826542	0.3017524004781972	0.0500690721870352
0.1334950372893031	0.8009231288186829	0.0496621889304029
0.3827272954166436	0.3005078883358245	0.0506288793080293
0.3820297573031504	0.8004398738643026	0.0504145271181285
0.6340323845238783	0.3017533002015908	0.0499263931538786
0.6337187505536739	0.8022263707481222	0.0505746840608032
0.8835345141383049	0.3031157628659938	0.0494893926006424
0.8836136045638407	0.8033065345065799	0.0501999332968269
0.4943760973651349	0.2465697741685271	0.4577975264723203
0.5893506267790590	0.7213268428099183	0.4711283867617568
0.4937704768691353	0.2277887566835441	0.4112902831832801
0.5938449831055468	0.7112658309073204	0.4250747093096486

Cu(111) *OCCOH

1.0000000000000000

10.2671904600000001 0.0000000000000000 0.0000000000000000

-5.1335952300000001 8.8916477700000005 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C H

64 2 2 1

Direct

0.9862249815357512	0.1213949134468944	0.3224912995359256
0.9880605128271989	0.3745233075629829	0.3239890452407920
0.9924763125202398	0.6260359475857893	0.3232934464703993
0.9917145744146691	0.8751534562979257	0.3232714718664388
0.2376536769739686	0.1211309245323752	0.3226926226528695
0.2271251329643939	0.3611415865345581	0.3270198366274235
0.2436617675863921	0.6225686834901448	0.3286137485815607
0.2407480868441283	0.8745641111436298	0.3229990247990231
0.4908964868947289	0.1270915854649652	0.3228737241775321
0.4851526641742333	0.3795873595382596	0.3279180369215725
0.5052652936870808	0.6408042992331733	0.3265853895188681
0.4928739735160384	0.8795933403134165	0.3241288231401777
0.7402129564197681	0.1269905771082090	0.3236999976435304
0.7391553790728275	0.3759065247120702	0.3229724324239748
0.7449723168454087	0.6285157520606942	0.3229356933409856
0.7459205942559337	0.8803482924769216	0.3223923292888359
0.1575257551308627	0.2094335525548910	0.2413153732531880
0.1594017795262344	0.4575164309767205	0.2419358948166092

0.1613578743106768 0.7053277499058659 0.2427835299478464
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0.4922916748856873	0.6249227894766424	0.0768917988430543
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0.7417641253015492	0.1252960338510135	0.0768661551790703
0.7414440652107332	0.3750972764935547	0.0769637699490686
0.7423202747553848	0.6252228201650277	0.0769369620492311
0.7426131806308061	0.8752049642606360	0.0769478918019898
0.4267475734291684	0.4113757346668837	0.4301005592754862
0.3113944594802155	0.5984519909727688	0.4354255512308689
0.3931147844532396	0.4533045611462668	0.3878731682698309
0.3327732812492331	0.5551356651621061	0.3856898177989631
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Cu(111) *COCO

1.0000000000000000

10.2671904600000001 0.0000000000000000 0.0000000000000000

-5.1335952300000001 8.8916477700000005 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C

64 2 2

Direct

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0.9914427078596906	0.6247187698428704	0.3233612357365728
0.9926111712213338	0.8753003053935406	0.3235524362905651
0.2409164488821994	0.1252082515887439	0.3262157021535678
0.2382306200302314	0.3719528779242994	0.3262932774570869
0.2399884847235842	0.6234190375597731	0.3267616647551533
0.2401155711577091	0.8759702905094653	0.3229239017445621
0.4929761584161537	0.1249345480556704	0.3228811478680184
0.4912689438051208	0.3773345033428105	0.3264866197422249
0.4951058626198649	0.6286114736742003	0.3257031253739442
0.4917836542513045	0.8763134213106438	0.3260123658449544
0.7410670488378399	0.1258229297410334	0.3230281625246106
0.7416539247914213	0.3759544986384877	0.3226875860588239
0.7428081493202499	0.6247558922923506	0.3233910802032724
0.7445920333298898	0.8771158174719347	0.3225934617661541
0.1593383374333719	0.2092888667363436	0.2413830565574164
0.1609389038124216	0.4588180758959386	0.2427620292656588
0.1596992063403845	0.7075800884683225	0.2420865784299198

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0.3240945907850601 0.5414786620308661 0.1597196886483360
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Cu Twin Boundary Concave In-plane *OCCOH

1.0000000000000000

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0.0000000000000000 15.4287675854564803 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C H

180 2 2 1

Direct

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0.6898354951554333 0.9718891566637055 0.3405992406473864
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0.9137968792440569 0.4719401547001013 0.5033744653671537
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Cu Twin Boundary Concave In-plane *COCO

1.0000000000000000

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0.0000000000000000 15.4287675854564803 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C

180 2 2

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Cu Twin Boundary Convex In-plane *OCCOH

1.0000000000000000

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0.0000000000000000 15.4287675854564803 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Cu O C H

180 2 2 1

Direct

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0.3547210528011626	0.2220532580134006	0.5215667796020561
0.3547909116978186	0.3885688976748747	0.5229495394888556
0.3540257293499148	0.5560963519635933	0.5229282823296016
0.3536538276177520	0.7227368985777014	0.5213574598198768
0.3548114218331881	0.8888678285264873	0.5212039601079593
0.5289206227834191	0.0555106159772576	0.3834338522779053
0.5288874360885779	0.2218447309974463	0.3835212066673073
0.5288805871785323	0.3892642557878948	0.3842467241789603
0.5302431342573447	0.5567607304917733	0.3853890703932056
0.5301895645190563	0.7217120753371723	0.3843090551263719
0.5288130818214958	0.8894024927143322	0.3832906795514076
0.6922631825362349	0.0557213849465284	0.2356614064030374
0.6920854102088686	0.2221153382319914	0.2360046577526994
0.6923432814493595	0.3888139324653839	0.2363071695441751
0.6921911097768402	0.5556530047758134	0.2363988904168259
0.6919486700171793	0.7223034610196376	0.2362069893235275
0.6923263153726037	0.8892028432384176	0.2356411512141594
0.6287486607017927	0.6485707475447668	0.5802782700174243
0.4960410028794235	0.4727457023547729	0.5825634887994379
0.6244507559503263	0.6460252183270291	0.5341359197664817
0.4507417915786721	0.4728900819250983	0.5441377065862306

Cu Twin Boundary Concave Out-of-plane *OCCOH

1.0000000000000000

15.3961024381587794	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.4287675854564803	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Cu O C H

180 2 2 1

Direct

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0.9425648168053287	0.4711122970481408	0.4582317911995389

0.9454764388762110 0.6398577792516652 0.4561042751813718
0.9483059932405487 0.8057945596561310 0.4544207481599569
0.9447920594961192 0.9710263119382925 0.4535621787355170
0.1101466846168402 0.1370044293646802 0.3123204829493034
0.1100111681395369 0.3054137778878928 0.3130489277452795
0.1092780742687352 0.4722878915153705 0.3123432163536965
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0.8592721563076561 0.3878571200026026 0.2345012719828861
0.8598477860969319 0.5540075837091853 0.2341814146671434

0.8603359930181810	0.7207188079618024	0.2334093435778480
0.8597570548434709	0.8875129148022260	0.2331364342302155
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0.3610471050400284	0.7215922527379953	0.5215908713393345
0.3628500899635453	0.8844270705220506	0.5210234069737298
0.5298103867677305	0.0553915012111747	0.3827856847358154
0.5303182699455065	0.2218415403293110	0.3833781355906229
0.5308251221695275	0.3876109227672022	0.3837478336236447
0.5297851746561343	0.5534730059227281	0.3806415826427432
0.5293899496675520	0.7212778944722562	0.3795214886670391
0.5298139930796493	0.8893338367315010	0.3802109787979281
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0.6934105067679430	0.2219201689615939	0.2353375525521009
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0.6942563233911284	0.5535396949364584	0.2356593345512980
0.6945376500435775	0.7214745167875604	0.2339357683985978
0.6934694963781233	0.8883716010169991	0.2345502710541074
0.8727116886021842	0.2794843039750104	0.5640235786048807
0.8636914634578428	0.4567247058437549	0.5626811545291152
0.8690612482187684	0.3218988733224043	0.5160524461201357
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Cu Twin Boundary Concave Out-of-plane *COCO

1.0000000000000000

15.3961024381587794	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.4287675854564803	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Cu O C

180 2 2

Direct

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0.9461554271170062	0.6418171931529508	0.4539409212539357
0.9474272366455497	0.8059841873663798	0.4551965421501626
0.9429620373235805	0.9721186598569013	0.4548233846723762
0.1084575842593725	0.1385501329994657	0.3136572808059465
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0.1085064607928138 0.4730343887239473 0.3122198583819651
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Cu Twin Boundary Convex Out-of-plane *OCCOH

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Cu O C H

171 2 2 1

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Cu Twin Boundary Convex Out-of-plane *COCO

1.0000000000000000

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Cu O C

171 2 2

Direct

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